Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 349 °C

Global applicability domain: Outside

Local applicability domain index: 2.96e-01

Confidence level: 6.78e-01

Nearest Neighbors from the Training Set

Image not found
Benfluralin
Measured: 370
Predicted: 349

Image not found
Pendimethalin
Measured: 330
Predicted: 335

Image not found
2,4,5-Trinitrotoluene
Measured: 300
Predicted: 309

Image not found
2,3,4-Trinitrotoluene
Measured: 301
Predicted: 309

Image not found
Carfentrazone-ethyl
Measured: 353
Predicted: 350